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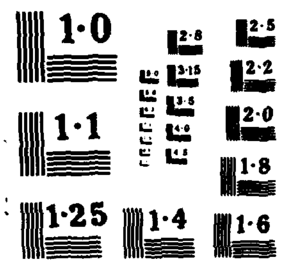
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TECHNICAL MEMORANDUM
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CHARACTERISTICS OF AN EBERT MONOCHROMATOR FOR AN INFRARED SPECTROMETER IN THE WAVELENGTH RANGE 1 μm TO 15 μm

S.S. TI

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CHARACTERISTICS OF AN EBERT MONOCHROMATOR FOR AN INFRARED SPECTROMETER IN THE WAVELENGTH RANGE 1 μm TO 15 μm

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S U M M A R Y

An Ebert monochromator of a UV spectroradiometer is to be adapted for use in an IR spectrometer in the wavelength range 1 μm to 15 μm. The adaptation requires a set of respecified data based on theoretical considerations of the geometrical feature of the monochromator. The basic principles are outlined and the new specification is summarised.

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1. INTRODUCTION

An Ebert monochromator-based UV spectroradiometer was designed and constructed in ERL in early 1980, and was shown to perform satisfactorily within the specifications in the wavelength range of 200 nm to 300 nm. Two of the main features of the UV spectroradiometer are its robustness and easy portability which are the imperative features for an instrument to be used for field trials and measurements.

In view of cost and time saving, it has been decided to adapt this spectroradiometer for measurement of IR radiation in the wavelength range of 1 µm to 15 µm.

The modification and adaptation procedure will be based on maximising the use of existing components, especially the mechanical parts. Redesign and construction of some components will, however, be inevitable.

The conversion of this UV spectrometer designed for the narrow range of 200 nm to 300 nm to an IR spectrometer usable in the wider range of 1 µm to 15 µm requires a set of respecified data for the Ebert monochromator. Such respecification will involve theoretical consideration of geometrical features in the Ebert monochromator.

This respecified monochromator will be used in the IR spectrometer currently under construction for the measurement of the emission spectra of flames.

2. GEOMETRY OF EBERT MONOCHROMATOR

The main feature of the Ebert monochromator is shown in figure 1.

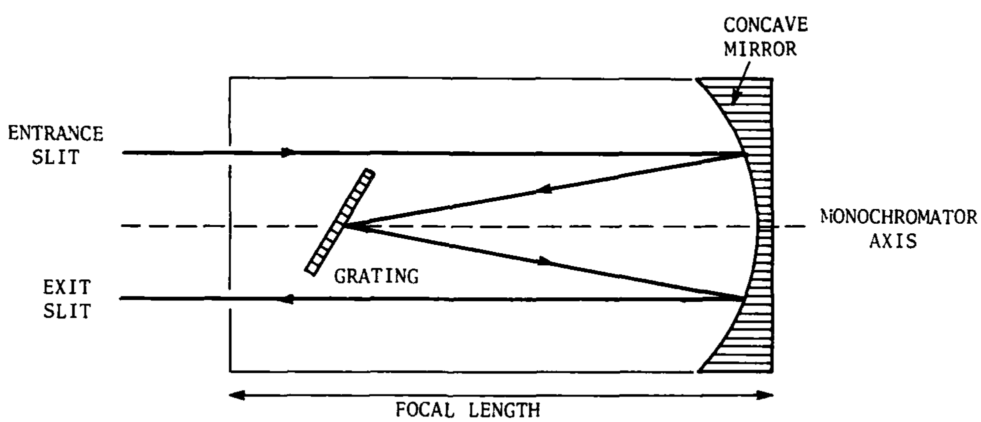
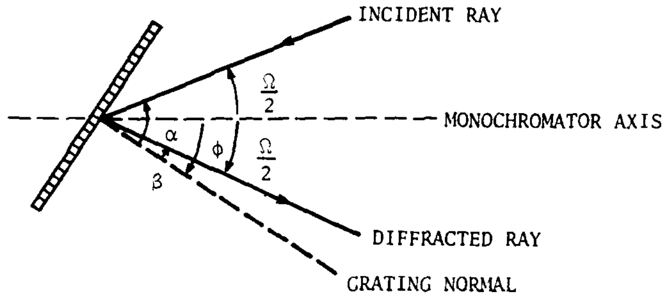


Figure 1. Geometry of the Ebert monochromator

Figure 2 below shows the ray angles at the grating surface as seen from the mirror:



α, the incident angle, is defined as the angle between the grating normal and the incident ray;
β, the diffraction angle is the angle between the grating normal and the diffracted ray;
ϕ, the grating angle, is the angle between the monochromator axis and the grating normal; and
Ω, the Ebert angle, is the angle between the incident ray and the diffracted ray.

Figure 2. Ray angles at the diffraction grating

From figure 1, it is obvious that consideration has to be given to the following:

(a) the characteristics of the diffraction grating to be used;

(b) the concave mirror which collimates and focuses;

(c) the placement of the grating; and

(d) the entrance and exit slits.

To facilitate subsequent discussion, several notations will be introduced at this stage:

For Grating:

d : grooves or lines separation distance (mm).
dg : diameter or equivalent diameter (mm).
Ag : area of grating surface (mm^2).

For Concave Mirror:

f : focal length (mm).
d_{cm} : diameter of the clear aperture of concave mirror, or simply length of mirror (mm).

For Slits:

w : width of slits (mm).
s : length of slits (mm).

$\bar{w}$: angular slit width, defined as $\frac{w}{f}$.

$\bar{s}$: angular slit length, defined as $\frac{s}{f}$.

ℓ : separation distance of the entrance and exit slits.

3. CHOICE OF DIFFRACTION GRATING

A diffraction grating is the dispersive device in the monochromator unit and its choice depends on, among others, two important factors:

(a) resolving power, and

(b) throughput.

These are discussed below:

3.1 Resolving power

The *resolving power (R) of a monochromator* is defined as

$$R = \frac{\lambda}{\Delta\lambda} \tag{1}$$

where λ is the wavelength of the incident radiation, and $\Delta\lambda = \lambda_1 - \lambda_2$, λ_1 and λ_2 being two wavelengths about λ which the monochromator is capable of resolving spectroscopically.

The resolving power of a grating is given by

$$R = mN \tag{2}$$

where m is the order of diffraction and N is the total number of grooves (lines) on the grating. For example for $\lambda = 10$ µm, $\Delta\lambda = 0.02$ µm and $m = 1$, $N = 500$.

To achieve a resolving power of 500, at least 500 grooves of the diffraction grating must be illuminated.

3.2 Throughput, G

The throughput of a monochromator, which depends on the groove density and the area of the grating used, can be expressed as(ref.1):

$$G = \frac{m \bullet d\lambda}{d \bullet \cos\beta} \bullet Ag \bullet \cos\left(\phi + \frac{\Omega}{2}\right) \bullet \bar{s} \tag{3}$$

which is similar to Jacquinot's flux output, F', at wavelength λ and using an unblazed grating:

$$F' \alpha \frac{\cos\left[\sin^{-1}\left(\frac{\lambda}{2d}\right) + \frac{\Omega}{2}\right] \bullet \cos\left[\sin^{-1} \frac{\lambda}{2d} - \frac{\Omega}{2}\right]}{d \bullet \cos^{2}\left[\sin^{-1}\left(\frac{\lambda min}{2d}\right) - \frac{\Omega}{2}\right]}$$

$$= k\ (\lambda, d) \qquad (4)$$

λ min here denotes the shortest wavelength considered.

A plot of $k(\lambda,d)$ versus λ, as shown in figure 3 suggests that the best throughput for an unblazed grating in the wavelength range of 6.0 μm to 15μm is given by the unblazed grating of 100 lines mm^{-1}. For shorter wavelength regions, gratings of groove density of 300 lines mm^{-1} and 200 lines mm^{-1} are suitable for spectral ranges of 1.8 μm to 4.5 μm, and 2.9 μm to 7.5 μm, respectively.

The overall throughput for each grating over the spectral range of interest (λ_1 to λ_2) is given by:

$$P\ (d) = \int_{\lambda_1}^{\lambda_2} k\ (\lambda, d)\ d\lambda \qquad (5)$$

The P(d) values obtained support the choice of gratings mentioned above.

For a resolving power of 500, at least 1.7 mm, 2.5 mm and 5.0 mm of the gratings of groove density 300 lines mm^{-1}, 200 lines mm^{-1} and 100 lines mm^{-1}, respectively, must be irradiated.

The typical square grating manufactured by Oriel Corporation has dimensions which will produce the specified resolution. However, the actual resolving power is determined also by other optical components in the system.

In general, the use of a grating of larger area will increase the sensitivity and the throughput of the monochromator but at the expense of increasing cost.

In order to save cost and to avoid delay, three gratings currently available will be used to cover the spectral ranges of interest, as indicated below:

7.7 μm to 15 μm : a circular grating of diameter 80 mm and of 75 lines mm^{-1}, blazed at 10 μm.

2.7 μm to 6.5 μm : a square grating of side 40 mm and of 300 lines mm^{-1}, blazed at 5.4 μm.

1.5 μm to 4.0 μm : a square 40 mm x 40 mm grating of 450 lines mm^{-1}, blazed at 3 μm.

Unless otherwise stated, the subsequent data calculated will be based on the circular grating of 80 mm diameter.

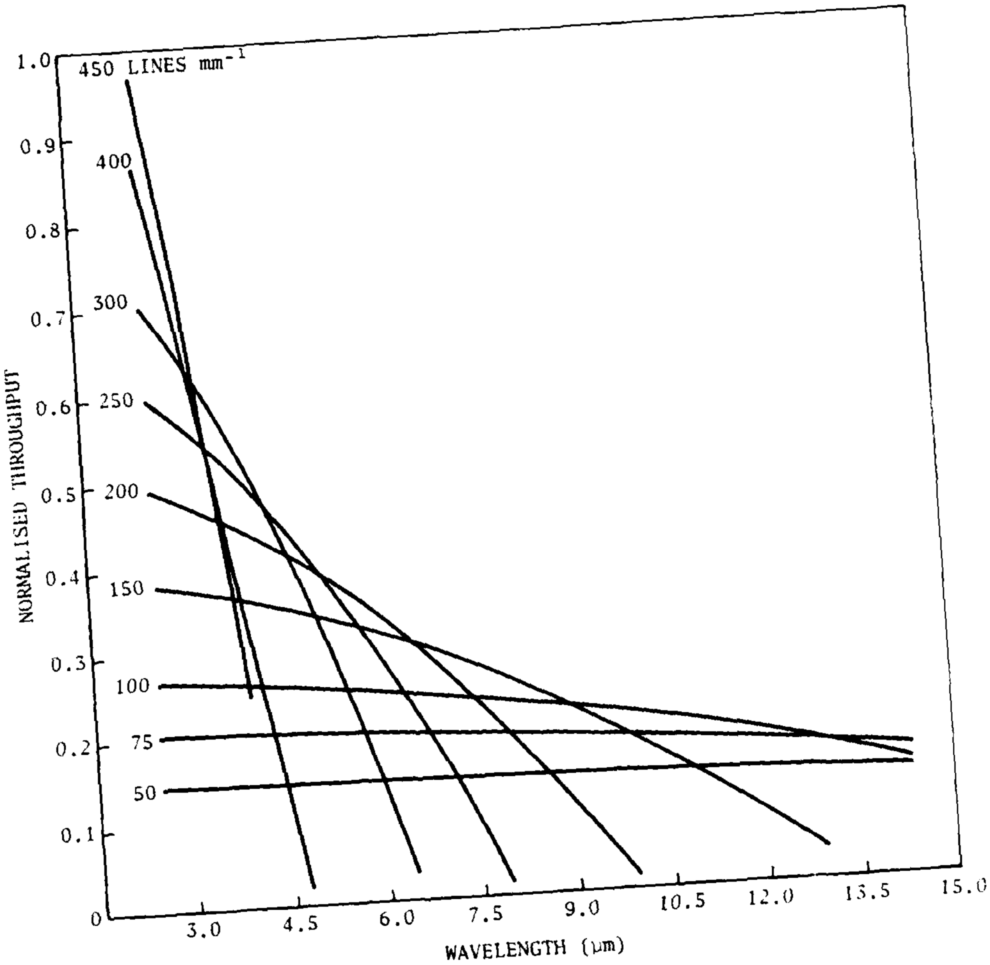


Figure 3. Throughput as a function of wavelength for different unblazed diffraction gratings

4. FOCAL LENGTH OF CONCAVE MIRROR

The concave mirror is used for collimating the incident rays and focusing the diffracted rays. The focal length and the f numbers of the monochromator must be selected to achieve a maximum throughput G.

The f number, F, of a monochromator is defined as

$$F = \frac{f}{dg} \tag{6}$$

From the equation (3) on the throughput G, it can be seen that the first order diffraction of a given λ by a grating of area Ag and with a constant $d\lambda$, G is independent of F provided $\bar{s}$ remains constant.

Hence, the choice of f and F can be made to achieve a compromise between the physical size (decreases with f) and the resolution (increased with f).

It is to be noted that at small f numbers, spherical aberration and residual coma become significant.

For a small f number Ebert monochromator with acceptable image forming properties (angular spherical aberration $\leq \frac{1}{2}$ angular slit width), it has been derived that:

$$F \geq 2.5$$

Thus for a grating of 80 mm in diameter,

$$f \geq 200 \text{ mm}$$

For a square grating of side 40 mm, its equivalent diameter is 46 mm. Therefore

$$f \geq 58 \text{ mm}$$

From an economy point of view, the existing concave mirror of focal length of 350 mm will be retained.

5. DIMENSIONS OF SLITS

The dimensions of slits must be carefully selected to achieve the desired resolution and to reduce optical aberrations. They are discussed below:

5.1 Slit length and astigmatism

The major limitation on resolving power of a monochromator is the astigmatism produced when long straight slits are used. For astigmatism to be acceptable ($\leq\frac{1}{4}w$),

$$\frac{d\lambda}{d} > \frac{0.2 \cdot s}{f\,F^2},$$

and substituting for F,

$$\frac{d\lambda}{d} > \frac{0.2 \cdot s\ (dg)^2}{f^3} \tag{7}$$

Using equation (7), and for $d = \frac{1}{75}$ mm, dg = 80 mm and $d\lambda$ = 0.02 µm,

$$\frac{s}{f^3} < 1.1 \times 10^{-6}\ mm^{-2}$$

A tabulation of f, s, $\bar{s}$, and F is shown in Table 1.

TABLE 1. RELATIONSHIP BETWEEN f AND LIMITING VALUE OF s FOR ACCEPTABLE ASTIGMATISM

f (mm)	s (mm)	$\bar{s}$ (rad)	F
200	8.8	0.044	2.50
250	17.2	0.069	3.13
300	29.7	0.099	3.75
350	47.2	0.135	4.38
400	70.4	0.176	5.00
450	100.2	0.223	5.63
500	137.5	0.275	6.25

From Table 1, it is seen that if f = 350 mm the slit length must be less than 47.2 mm for astigmatism to be acceptable. The factors of 12 and 18 are to be used respectively in calculating the slit length for acceptable astigmatism for the 300 lines mm^{-1} and 450 lines mm^{-1} gratings.

5.2 Slit length and resolution

Loss of resolution will occur if the image of the straight slit is curved due to the oblique incidence of the radiation on the mirror. To preserve the resolution, suitable curved entrance and exit slits can be used, but unfortunately they are difficult to manufacture.

A relationship exists, however, between the resolving power of a monochromator and length of straight slits in the following form(ref.1):

$$\left(\frac{s}{f}\right)^2 \leq \frac{4}{R} \tag{8}$$

for acceptable error ($\leq \frac{1}{2}$ slit length) in spectral imaging. For R = 500, $\bar{s} \leq$ 90 mrad.

Hence, the use of straight slits requires the angular slit length to be less than 90 mrad for the specified resolution to be attained.

The data in Table 1 provide a guide to the choice of focal length of the concave mirror and the corresponding slit lengths which satisfy the requirement on resolution.

Thus, so long as the straight slit lengths are kept below 30 mm, the use of the existing concave mirror of focal length 350 mm is satisfactory, although at the expense of slight reduction of throughput.

(c) Slit width and resolution

From the grating equation and the geometry in figure 2, it can be derived that the resolution of a monochromator relates to the slit width by

$$w = \frac{f \bullet d\lambda}{d \bullet \cos\left(\sin^{-1}\left(\frac{\lambda}{2d}\right) - \frac{\Omega}{2}\right)} \tag{9}$$

For $f = 350$ mm, $d\lambda/\lambda = 0.002$ and $\Omega/2 = 8.1°$ (see later), the slit widths for various wavelengths in the range of wavelengths 1 μm to 15 μm have been tabulated (Table 2).

TABLE 2. RELATIONSHIP BETWEEN SLIT WIDTH, WAVELENGTH AND GROOVE DENSITY FOR $d\lambda/\lambda = 0.002$ ($f = 350$ mm)

λ(μm)	1.5	2.5	3.5	4.0	4.4	2.7	3.7	4.7	5.7	6.7
w(mm)	0.48	0.88	1.53	2.26	4.97	0.59	0.86	1.23	1.89	7.56
d(mm)	1/450					1/300				

λ(μm)	7.5	8.5	9.5	10.5	11.5	12.5	13.5	14.5
w(mm)	0.40	0.45	0.51	0.57	0.63	0.70	0.77	0.84
d(mm)	1/75							

The setting of slit width corresponding to the other resolution at the above wavelengths can be calculated using both the data in Table 2 and the equation

$$\frac{w_1}{w_2} = \frac{d\lambda_1}{d\lambda_2} \tag{10}$$

(d) Separation distance of entrance and exit slits (ℓ)

The entrance and exit slits of the Ebert monochromator are separated so that the associated rays from the mirror clear the diffraction grating. For the grating diameter of 80 mm, the separation must be greater than 80 mm.

The existing separation distance of 92 mm is satisfactory and will be retained. It is to be noted that the separation distance of slits and the position of grating determine the Ebert angle, Ω.

From Figures 1 and 2, it is clear that

$$\tan\frac{\Omega}{2} = \frac{(92/2)}{325}, \text{ and}$$

$$\frac{\Omega}{2} = 8.1^\circ$$

Note: the grating is 325 mm from the mirror.

The Ebert angle is related to the grating angle by

$$\alpha = \emptyset + \frac{\Omega}{2} \tag{11}$$

which plays a role in determining the dispersion of radiation as is evident from the basic grating equation:

$$\sin\alpha + \sin\beta = \frac{m\lambda}{d} \tag{12}$$

and its derived form corresponding to Ebert geometry:

$$2d \sin\emptyset \cos\frac{\Omega}{2} = m\lambda \tag{13}$$

6. PLACEMENT OF DIFFRACTION GRATING

To have a straight slit imaged as a straight slit on a curved focal surface, the diffraction grating must be positioned between 0.846 and 0.960 of the distance from the mirror to the slit plane.

Presently, the grating is at 0.92 of the distance from the mirror to the slit plane (325 mm) and this allows an adequate range of grating angles up to 38°.

7. MONOCHROMATION OF DIFFRACTED RADIATION

Several different wavelengths may simultaneously satisfy the grating equation at a given grating angle, giving rise to various orders of diffraction.

In the Ebert monochromator, for a relatively narrow range of wavelengths, it is possible to choose a suitable grating and a concave mirror of suitable size so that only the first order diffracted radiation will be focused on the exit slit. However, for the larger range of IR wavelengths of interest, often both first and second order diffracted radiation will be focused on the exit slit simultaneously.

The use of suitable band pass filters will resolve this difficulty and the filter characteristics which are required may be determined as follows:

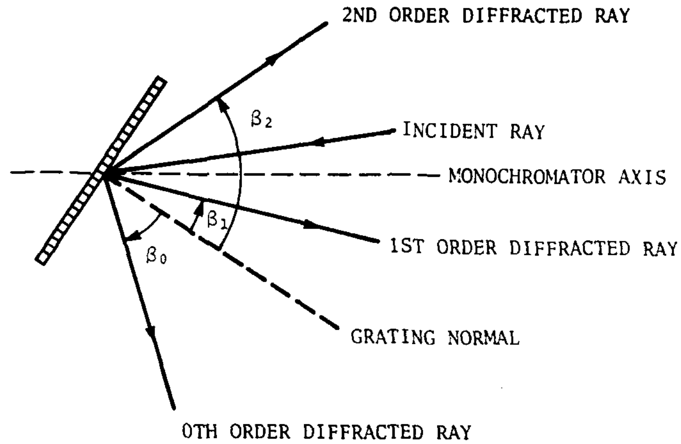


Figure 4. Multiple diffraction of radiation at grating surface

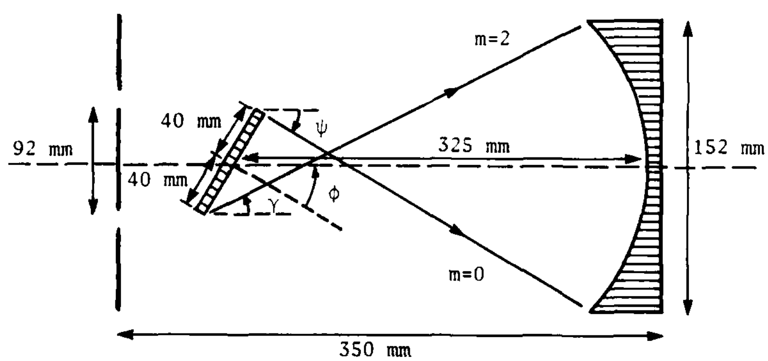


Figure 5. Geometry of $m \neq 1$ diffraction

Referring to figures 4 and 5, β_0 and β_{+2} denote, respectively, the zeroth order and second order diffracted angles. ψ and γ are the angles the zeroth order and second order diffracted rays make with the monochromator axis, respectively. It is evident that the m = 0 and m = 2 diffracted rays will be focused onto the exit slit if they strike the mirror.

Two conditions arise in order to avoid this situation:

(i) The m = +2 diffracted ray from the shortest wavelength at the largest grating angle must not strike the mirror.

ie

$$\beta_{+2} - \phi > \gamma, \text{ and}$$

(ii) the m = 0 diffracted ray from the largest wavelength at the smallest grating angle must not be incident on the mirror.

ie

$$\beta_0 + \phi > \psi$$

From the geometry in figure 5, γ and ψ are given by

$$\gamma = \tan^{-1} \frac{152/2 + 40 \cos\phi}{325 + 40 \sin\phi}, \tag{14}$$

and

$$\psi = \tan^{-1} \frac{152/2 + 40 \cos\phi}{325 - 40 \sin\phi}, \tag{15}$$

ϕ can be found from equation (13) and β from equation (12).

Using equations (12), (13), (14) and (15), and for a set of selected gratings and band pass filters, the corresponding effective ranges of first order pass bands have been calculated (see Summary).

8. SUMMARY OF MONOCHROMATOR CHARACTERISTICS

The data discussed in the preceding sections are collected here for ease of reference. They are the specifications of the Ebert monochromator to be used in constructing the 1 μm to 15 μm IR spectroradiometer for measuring the emission spectra of flames.

(a) Concave mirror

f : 350 mm
d_{cm} : 152 mm

(b) Gratings (Oriel)

	BLAZED AT (3 μm)	**BLAZED AT (5.4 μm)**	**BLAZED AT (10 μm)**
d :	1/450 mm	1/300 mm	1/75 mm
dg :	23 mm	23 mm	80 mm
Useable range :	1.43 μm to 4 μm	2.74 μm to 6.5 μm	7.7 μm to 15 μm
Distance from mirror :	325 mm		

(c) Slit length

$$\text{Maximum} \quad 30 \text{ mm for } \frac{d\lambda}{\lambda} = 0.002$$

(d) Resolution and slit width

$$\frac{w_1}{w_2} = \frac{d\lambda_1}{d\lambda_2} \tag{16}$$

RELATIONSHIP BETWEEN SLIT WIDTH, WAVELENGTH AND GROOVE DENSITY
FOR $\Delta\lambda/\lambda = 0.002$ (f = 350 mm)

λ(μm)	1.5	2.5	3.5	4.0	4.4	2.7	3.7	4.7	5.7	6.7
w(mm)	0.48	0.88	1.53	2.26	4.97	0.59	0.86	1.23	1.89	7.56
d(mm)	$\frac{1}{450}$					$\frac{1}{300}$				

λ(μm)	7.5	8.5	9.5	10.5	11.5	12.5	13.5	14.5
w(mm)	0.40	0.45	0.51	0.57	0.63	0.70	0.77	0.84
d(mm)	$\frac{1}{75}$							

(e) Gratings, filters and effective pass bands

Gratings (Oriel)	Filter pass bands (Oriel)	Effective pass bands (for 1st order diffraction)
450 1 mm^{-1} (3 μm)	1.2 μm to 2.0 μm 1.8 μm to 3.0 μm 2.7 μm to 4.5 μm	1.43 μm to 2.0 μm 1.83 μm to 3.0 μm 2.7 μm to 4.0 μm (*)
300 1 mm^{-1} (5.4 μm)	2.7 μm to 4.5 μm 3.8 μm to 6.5 μm	2.74 μm to 4.5 μm 3.8 μm to 6.5 μm (*)
75 1 mm^{-1} (10.0 μm)	6.0 μm to 10.0 μm 9.0 μm to 15.0 μm	7.7 μm to 10.0 μm 9.7 μm to 15.0 μm

(*) Theoretical values are 2.16 μm to 4.0 μm and 3.5 μm to 6.5 μm.

(f) Grating angles, ϕ

Gratings	λ	ϕ(**)
450 1 mm^{-1} (3 μm)	1.43 μm 2.0 μm 1.83 μm 3.0 μm 2.7 μm 4.0 μm	19.0° 27.0° 24.6° 43.0° 37.9° 65.4°
300 1 mm^{-1} (5.4 μm)	2.74 μm 4.5 μm 3.8 μm 6.5 μm	24.5° 43.0° 35.2° 80.0°
75 1 mm^{-1} (10 μm)	7.7 μm 10.0 μm 9.7 μm 15.0 μm	17.0° 22.3° 21.6° 34.6°

(**) For the circular grating of 80 mm diameter, the maximum grating angle allowed, as imposed by the geometry, is 38°

REFERENCES

No.	Author	Title
1	Johnson, R.P.	"A High Performance Ultraviolet Spectroradiometer". Thesis, Master of App Sc SAIT, (1980), and references therein

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